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Numerical Solution of First Order Stiff Ordinary Differential Equations using Fifth Order Block Backward Differentiation Formulas

(Penyelesaian Berangka bagi Persamaan Pembezaan Biasa Kaku Peringkat Satu Menggunakan Blok Formula Beza ke Belakang Peringkat Lima)

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ABSTRACT

This paper describes the development of a two-point implicit code in the form of fifth order Block Backward Differentiation Formulas (BBDF(5)) for solving first order stiff Ordinary Differential Equations (ODEs). This method computes the approximate solutions at two points simultaneously within an equidistant block. Numerical results are presented to compare the efficiency of the developed BBDF(5) to the classical one-point Backward Differentiation Formulas (BDF). The results indicated that the BBDF(5) outperformed the BDF in terms of total number of steps, accuracy and computational time.

Keywords: Block method; ordinary differential equation

ABSTRAK

Kertas ini membincangkan pembentukan kod tersirat dua titik dalam bentuk Blok Formula Beza Ke Belakang peringkat lima (BBDF(5)) bagi menyelesaikan Persamaan Pembezaan Biasa (PPB) kaku peringkat pertama. Kaedah ini mengira penyelesaian penghampiran dua titik serentak dalam jarak blok yang sama. Keputusan berangka diberi untuk membandingkan kaedah BBDF(5) dengan kaedah Formula Beza Ke Belakang klasik (BDF). Keputusan kajian menunjukkan bahawa BBDF(5) mengatasi BDF dalam hal jumlah langkah, kesalahan maksima dan masa pengkomputeraan.

Kata kunci: Kaedah blok; persamaan pembezaan biasa

INTRODUCTION

In this paper we are interested in the numerical solution of Initial Value Problems (IVPs) for first order stiff Ordinary Differential Equations (ODEs) of the form

$$y'_i = f_i(x,y), \qquad y(a) = \alpha, \qquad i = 1,2,\ldots,s, \tag{1}$$

where

$y(x) = (y_1, y_2, \ldots, y_s)^T$ and $\alpha = (\alpha_1, \alpha_2, \ldots \alpha_s)^T$ in the interval $[a,b]$.

Previous works on block methods for solving (1) are given by Rosser (1967), Chu and Hamilton (1987) and Fatunla (1990), to name a few. The block method produced numerical solutions with less computational effort as compared to nonblock method (see Majid (2004)). This is because the block method calculated more than one solution simultaneously. The block method consists of a number of points in each block, depending on the structure of that block. Voss and Abbas (1997) proposed one-step fourth-order block method and it was shown that the method can be paralleled as further research to enhance the efficiency. The definition of block method which have been defined by Voss and Abbas (1997), which is if $k \geq 1$ is the block size, a block of solutions can be represented by the vector $Y_i = (y_{n+1}, y_{n+2}, \ldots, y_{n+k})^T$ with yn+j($1 \leq j \leq k$), the generated solution at $x_{n+j} = jh$, where x_n is the right-hand end point of the preceding block and h is the step size.

Ibrahim et al. (2007) derived a new block method which is called the Block Backward Differentiation Formula (BBDF) to solve stiff ODEs. The BBDF is computed two points simultaneously in each block using x_{n-1} and x_n as the backvalues. As a result, the proposed method have improved the accuracy and required less computational time.

The focus in this paper is to extend the method derived by Ibrahim et al. (2007) to further improve the performance of the BBDF. In the next section, we will show the formulation of the fifth order Block Backward Differentiation Formulas which is denoted by BBDF(5) with fixed stepsize.

FORMULATION OF FIFTH ORDER BBDF METHOD (BBDF(5))

We consider the points x_{n-3}, x_{n-2}, x_{n-1} and x_n as the backvalues for calculating the values y_{n+1} and y_{n+2} simultaneously. The Lagrange polynomial P_k which has been used to interpolate the backvalues, is defined as:

$$P_k(x) = \sum_{j=0}^{k} L_{k,j}(x) y(x_{n+1-i}), \tag{2}$$

where

$$L_{k,j}(x) = \prod_{\substack{i=0 \\ i \neq j}}^{k} \frac{(x - x_{n+1-i})}{x_{n+1-j} - x_{n+1-i}}, \; j = 0, 1, \ldots, k.$$

In this method, the computation of approximation for y_{n+1} and y_{n+2} concurrently is by using one earlier block where there are two points in each block. We start by replacing $x = x_{n+1} + sh$ into (2) to formulate y_{n+1}, then we have:

$$\begin{aligned} P(x_{n+1} + sh) = {} & \frac{h(3+s)h(2+s)h(1+s)h(s)h(s-1)}{(-h)(-2h)(-3h)(-4h)(-5h)} y_{n-3} + \frac{h(4+s)h(2+s)h(1+s)h(s)h(s-1)}{(-h)(-2h)(-3h)(-4h)(h)} y_{n-2} + \\ & \frac{h(4+s)h(3+s)h(1+s)h(s)h(s-1)}{(-h)(-2h)(-3h)(h)(2h)} y_{n-1} + \frac{h(4+s)h(3+s)h(2+s)h(s)(s-1)}{(-h)(-2h)(3h)(2h)(h)} y_n + \\ & \frac{h(4+s)h(3+s)h(2+s)h(1+s)h(s-1)}{(-h)(4h)(3h)(2h)(h)} y_{n+1} + \frac{h(4+s)h(3+s)h(2+s)h(1+s)h(s)}{(h)(2h)(3h)(4h)(5h)} y_{n+2}. \end{aligned} \tag{3}$$

Subsequently, by differentiating (3) once with respect to s at the point $x = x_{n+1}$. On substituting s = 0, and equating $hf_{n+1} = hP'(x_{n+1})$, will produce the following formula for y_{n+1}:

$$y_{n+1} = -\frac{3}{65} y_{n-3} + \frac{4}{13} y_{n-2} - \frac{12}{13} y_{n-1} + \frac{24}{13} y_n - \frac{12}{65} y_{n+2} + \frac{12}{13} hf_{n+1}. \tag{4}$$

Similarly, applying the same steps as above and evaluating $s = 1$ to formulate y_{n+2}, hence will produce:

$$y_{n+2} = \frac{12}{137} y_{n-3} - \frac{75}{137} y_{n-2} + \frac{200}{137} y_{n-1} - \frac{300}{137} y_n + \frac{300}{137} y_{n+1} + \frac{60}{137} hf_{n+2}. \tag{5}$$

Therefore, the corrector is formulated as follows:

$$\left.\begin{aligned} &1) \quad y_{n+1} = -\frac{3}{65} y_{n-3} + \frac{4}{13} y_{n-2} - \frac{12}{13} y_{n-1} + \frac{24}{13} y_n - \frac{12}{65} y_{n+2} + \frac{12}{13} hf_{n+1} \\ &\text{and} \\ &2) \\ &\quad y_{n+2} = \frac{12}{137} y_{n-3} - \frac{75}{137} y_{n-2} + \frac{200}{137} y_{n-1} - \frac{300}{137} y_n - \frac{300}{137} y_{n+1} + \frac{60}{137} hf_{n+2} \end{aligned}\right\} (6)$$

The formulas (6) are fully implicit, so we need to derive the predictor to compute the starting values which are y_{n-3}, y_{n-2}, y_{n-1} and y_n. The future values for y_{n+2} and f_{n+1} are also obtained from the predictors. The predictor formula is constructed in the usual manner by interpolating the points x_{n-4} x_{n-3}, x_{n-2}, x_{n-1} and x_n. Next, we determined the order of the method given in (6).

ORDER OF THE METHOD

In this section, we will determine the order of the proposed method given in (6). We illustrate the definitions of the order for Linear Multistep Method (LMM) as given in Lambert (1991) using the following definitions:

Definition 1
The Linear Multistep Method (LMM) given by:

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f_{n+j}, \tag{7}$$

where α_j and β_j are constants subject to the conditions $\alpha_k = 1, | \alpha_0 | + | \beta_0 | \neq 0$.

Definition 2
The LMM (7) and the associated difference operator L defined by

$$L[z(x); h] := \sum_{j=0}^{k} [\alpha_j z(x + jh) - h\beta_j z'(x + jh)], \tag{8}$$

are said to be of order p if $C_0 = C_1 = \ldots = Cp = 0, C_{p+1} \neq 0$. The general form for the constant C_q is defined as:

$$C_q = \sum_{j=0}^{k} \left[\frac{1}{q!} j^q \alpha_j - \frac{1}{(q-1)!} j^{q-1} \beta_j \right] \quad q = 2, 3, \ldots, p+1. \tag{9}$$

The formulas in (6) can be written in general matrix form as follows:

$$\sum_{j=0}^{k} A_j Y_{n+j} = h \sum_{j=0}^{k} F_{n+j}, \tag{10}$$

where A_j and B_j are r by r matrices with elements $a_{l,m}$ and $b_{l,m}$ for $l, m = 1, 2, \ldots, r$. Since BBDF(5) is a block method, we extend the definition 2 in the form:

$$L[z(x); h] := \sum_{j=0}^{k} [A_j z(x + jh) - hB_j z'(x + jh)],$$

and the general form for the constant C_q is defined as:

$$C_q = \sum_{j=0}^{k} \left[\frac{1}{q!} j^q A_j - \frac{1}{(q-1)!} j^{q-1} B_j \right] \quad q = 2, 3, \ldots, p+1. \tag{11}$$

In order to apply the definitions, we need to rearrange the formulas given in (6) into the form given by equation (10). Then we implemented (11) into (6) in order to find the order of the formulas, hence we obtain $C_6 \neq 0$. Thus, we can conclude that our method is fifth order.

NUMERCIAL RESULTS

We will compare the BBDF(5) with classical one-point Backward Differentiation Formula (BDF) which is given as:

$$y_{n+1} = -\frac{3}{25}y_{n-3} + \frac{16}{25}y_{n-2} - \frac{36}{25}y_{n-1} + \frac{48}{25}y_n + \frac{12}{25}hf_{n+1}. \quad (10)$$

The following problems are solved numerically using the BBDF(5) and the BDF.

Problem 1

$$y' = -100\,(y - x^3) + 3x^2, \qquad x \in [0, 10],$$

where the initial condition, $y(0) = 0$, the eigenvalue is $\lambda = -100$ and $y = x^3$ is the exact solution (Brannan et al. 2007).

Source : Brannan and William (2007).

Problem 2

$$y'_1 = -2y_1 + y_2 + 2\sin x,$$

$$y'_2 = 998y_1 - 999y_2 + 999\,(\cos x - \sin x), \qquad x \in [0, 10],$$

where the initial condition, $y_1(0) = 2$, $y_2(0) = 3$, the eigenvalues are $\lambda_1 = -1$, $\lambda_2 = -1000$ and $y_1 = 2e^{-x} + \sin x$, $y_2 = 2e^{-x} + \cos x$ is the analytic solution

Source : Lambert (1991).

Problem 3

$$y'_1 = 198y_1 + 199y_2$$

$$y'_2 = -398y_1 - 399y_2 \qquad x \in [0, 5],$$

where the initial condition, $y_1(0) = 1$, $y_2(0) = -1$, the eigenvalues are $\lambda_1 = -1$, $\lambda_2 = -200$ and $y_1(x) = e^{-x}$, $y_2(x) = -e^{-x}$ is the analytic solution.

Source : Ibrahim *et al*. (2007).

Notations used in the following tables are:

BDF : classical one-point Backward Differentiation Formula
BBDF(5) : fifth order Block Backward Differentiation Formulas
H : step size
TS : the total number of steps
TIME : the time execution (μs)
MAXE : maximum error
AVE : average error

The calculation of error is given as:

$$ERROR_j = |\, y_{j(exact\ solution)} - y_{j(approximate)} |.$$

For maximum error, we compute using the formula which is defined as follows:

$$MAXE = \max_{1 \le j \le NS}\left(|\, y_{j(approximate)} - y_{j(exact\ solution)}\, |\right),$$

and the average error is defined as:

$$AVE = \frac{\sum_{j=1}^{NS} ERROR_j}{n},$$

where $n = \dfrac{(b-a)}{H}$, b is the end value of x and a is the initial value of x. The numerical results are tabulated in Table 1.

TABLE 1: Numerical results for problem 1 and 2

Problem	*H*	Method	TS	MAXE	TIME	AVE
1.	10^{-4}	BDF	100,000	5.99403e-005	431940	1.99801e-005
		BBDF(5)	50,000	1.19880e-004	24447	1.99800e-005
	10^{-6}	BDF	10,000,000	5.96096e-007	43164000	1.98650e-007
		BBDF(5)	500,000	1.19872e-006	2457650	1.99809e-007
	10^{-8}	BDF	100,000,000	1.55652e-007	4302530000	4.41561e-008
		BBDF(5)	50,000,000	5.48359e-008	247317000	8.54131e-009
2.	10^{-4}	BDF	100,000	8.38318e-004	599612	1.48119e-005
		BBDF(5)	50,000	1.02772e-004	50008	1.33710e-005
	10^{-6}	BDF	10,000,000	8.38225e-005	59762100	1.48078e-006
		BBDF(5)	500,000	1.02861e-006	5772230	1.33778e-007
	10^{-8}	BDF	100,000,000	8.38318e-007	5929610000	1.48119e-008
		BBDF(5)	50,000,000	6.77840e-009	589993000	5.10639e-010
3.	10^{-4}	BDF	100,000	7.33443e-005	103300	1.12283e-006
		BBDF(5)	50,000	7.32892e-005	22110	1.22720e-006
	10^{-6}	BDF	10,000,000	7.35743e-007	49983000	1.68444e-008
		BBDF(5)	500,000	2.51124e-008	2203750	4.11149e-009
	10^{-8}	BDF	100,000,000	7.33881e-008	4287873000	1.67792e-009
		BBDF(5)	50,000,000	2.88631e-010	190338000	3.15423e-012

Conclusion

Our results showed that BBDF(5) outperformed the BDF in terms of execution time, total number of steps and accuracy. Furthermore, BBDF(5) was more efficient at smaller stepsize as shown by the average error. Hence, the BBDF(5) is more efficient than BDF. Future research is in progress on extending the method using variable-step size.

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